



Increasing Selectivity and Sensitivity in Ion Mobility Spectrometry using Ion Beam Modulation

M. Todd Griffin; Jack E. Fulton, Jr.; Robert F. McAtee;

Chemical, Biological, and Explosives Detection Group
NSWC, Crane Division
Crane, IN 47522

Distribution Statement A - Approved for public release; distribution unlimited.



Report Documentation Page				Form Approved OMB No. 0704-0188	
Public reporting burden for the collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to a penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.					
1. REPORT DATE 01 OCT 2005		2. REPORT TYPE N/A		3. DATES COVERED -	
4. TITLE AND SUBTITLE Increasing Selectivity and Sensitivity in Ion Mobility Spectrometry using Ion Beam Modulation				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Chemical, Biological, and Explosives Detection Group NSWC, Crane Division Crane, IN 47522				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release, distribution unlimited					
13. SUPPLEMENTARY NOTES See also ADM001851, Proceedings of the 2003 Joint Service Scientific Conference on Chemical & Biological Defense Research, 17-20 November 2003. , The original document contains color images.					
14. ABSTRACT					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	18. NUMBER OF PAGES 18	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			



Chem/Bio/Explosive Detection



FACILITIES

- Unique 25,000 Sq. Ft. Chemical/Biological Detection Center
- Physical Plant Replacement Value of \$4.0M
- Specialized Chemical/Biological Detection Equipment with Replacement Value of \$5.0M
 - Thermal Collimators
 - Chemical Vapor Diagnostic Test Sets
 - Chemical Vapor Generators
 - Chemical Hazard Containment Room

CAPABILITIES

- Develop & Review Specifications
- Develop Procurement Technical Data Packages
- Contract for Products, Components or Services
- Acceptance Test New Systems
- Repair Chemical Detection Devices
- Provide On-Site Fleet Support and Training
- Initiate & Implement Engineering Change Proposals
- Provide Sustainment Logistics Support for New & Existing Systems
- Perform Failure Analysis
- Hold Navy Radioactive Material Handling Permit

PERSONNEL

- Highly Technical Workforce of 51 Professionals with Extensive Chemical/Biological/Explosive Detection Experience
- Skills Mix of Thermal Imagers, and IMS Expertise
- 19 Engineers and Scientists
- 32 Skilled Technicians/Logisticians/Equipment Specialists



Code 805D Customers

- Navy
 - Naval Sea Systems Command
 - Naval Special Warfare Command
 - Navy Inventory Control Point, Mechanicsburg
 - Navy Explosive Ordnance Disposal Units
 - Navy Construction Battalions
 - Office of Naval Research

- Other
 - Defense Threat Reduction Agency
 - Soldier, Biological, Chemical Command
 - Joint Program Office – Biological Defense



Code 805D Tasking

- Acquisition Engineering Support
- Production Acceptance Testing
- Installation & Fielding Support
- In-Service Engineering Support
 - Product Improvement Programs
 - Configuration Management- Hardware and Software
 - Intensified Leak Test Tracking for Radioactive Sources
- Depot Maintenance and Repair
- Support New Construction Ships
- Product Integration (System Design and Integration)

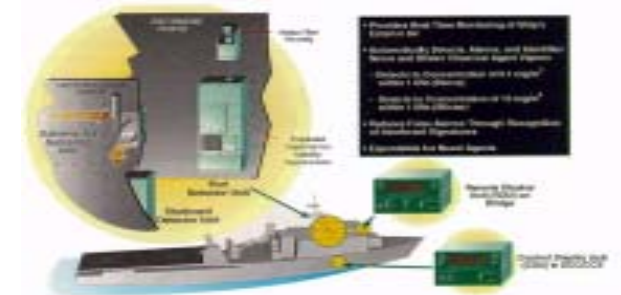
IMS in the Field



Automatic Chemical Agent Detection Alarm (ACADA)



Improved Chemical Agent Monitor (ICAM)



Improved Point Detection Sys. (IPDS)



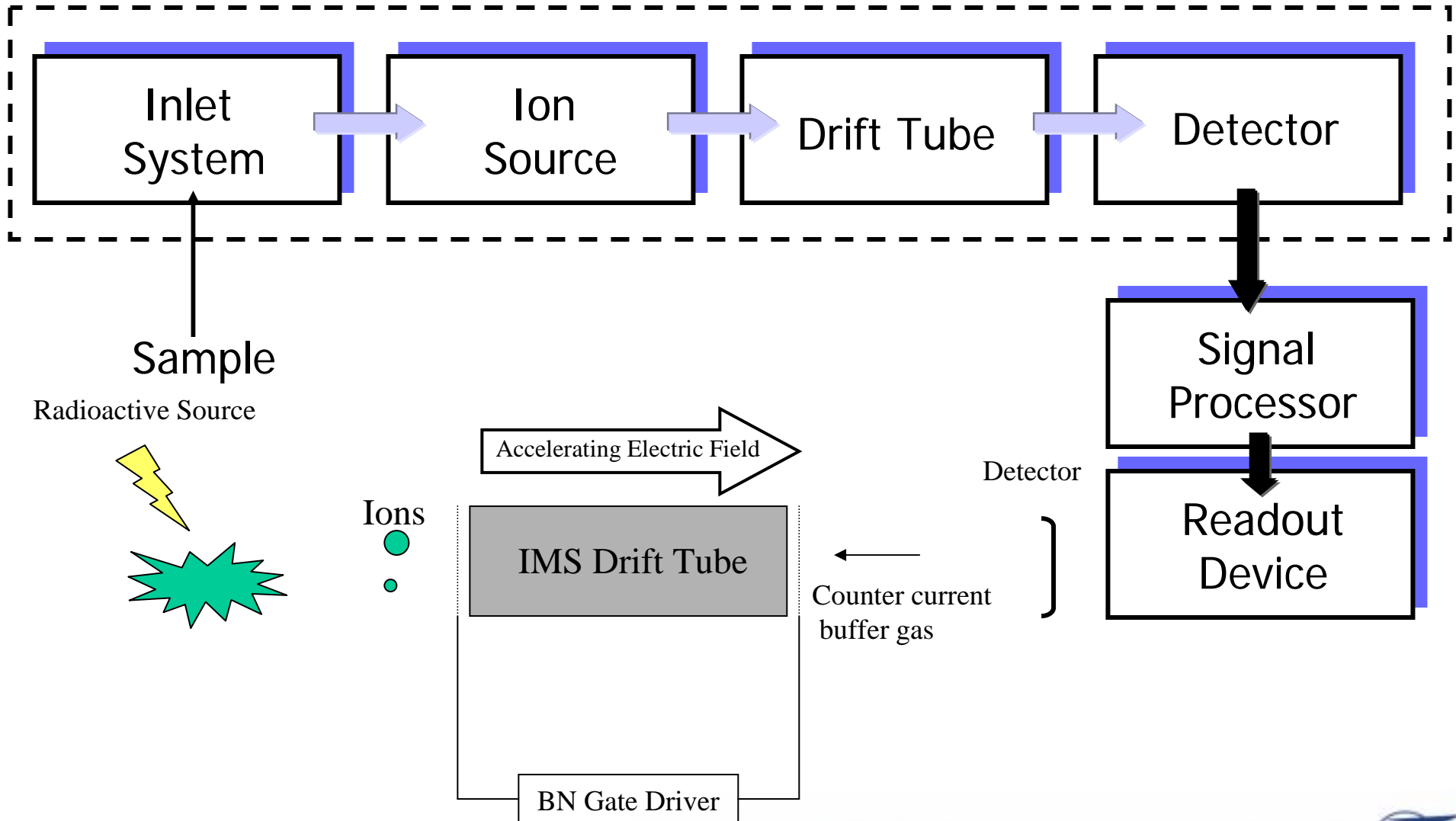
Shipboard ACADA



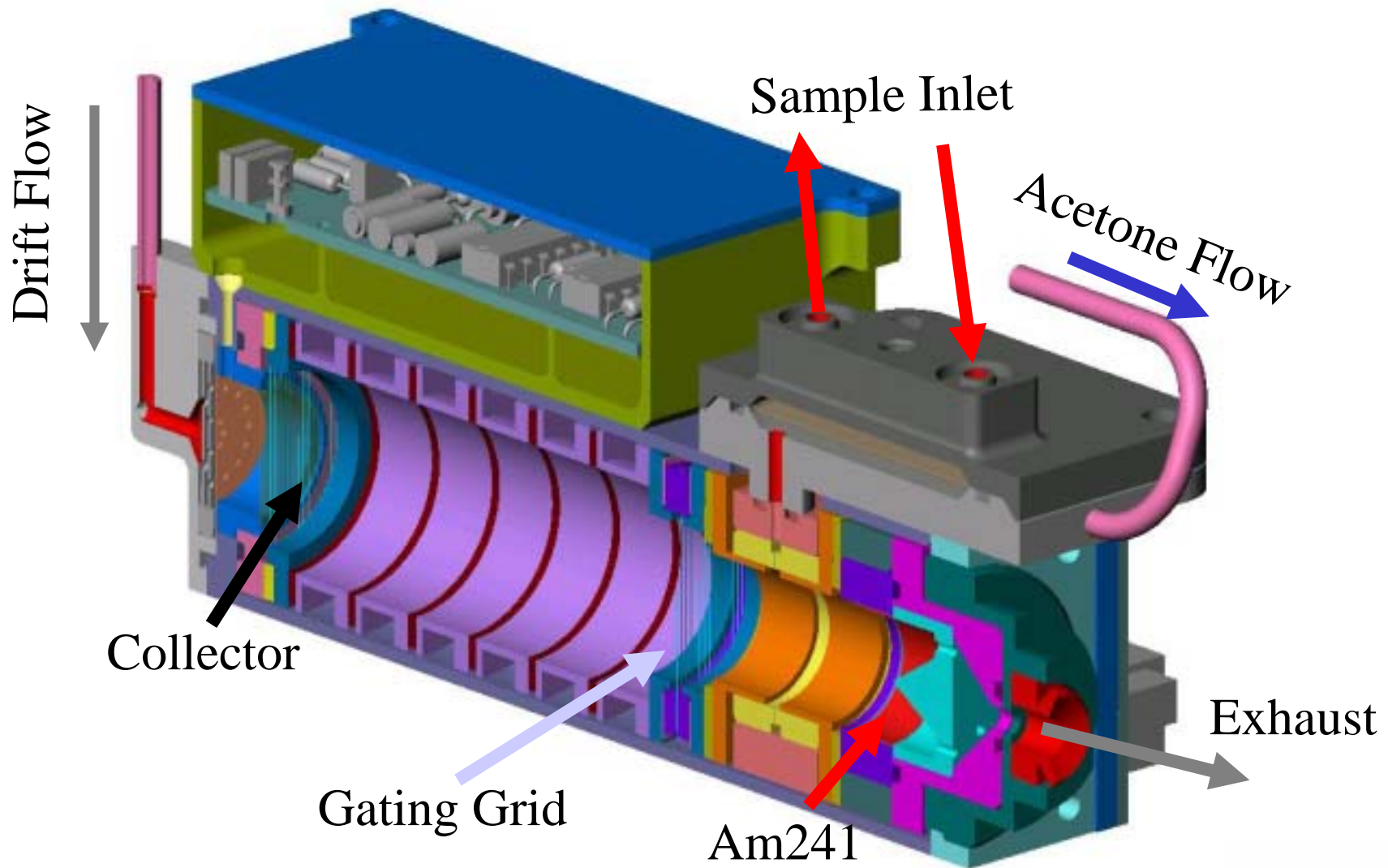
VaporTracer II (Explosives)

Ion Mobility Spectrometry: System Block Diagram

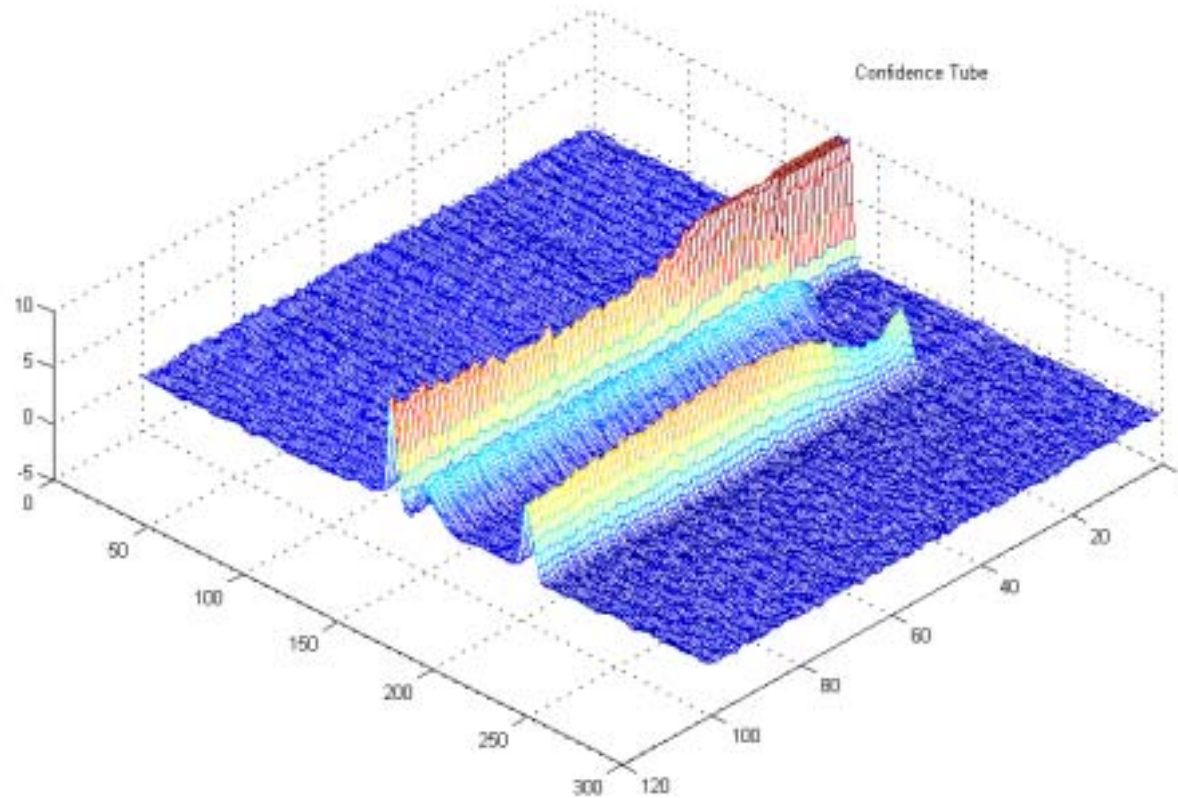
Atmosphere



Field Portable IMS System

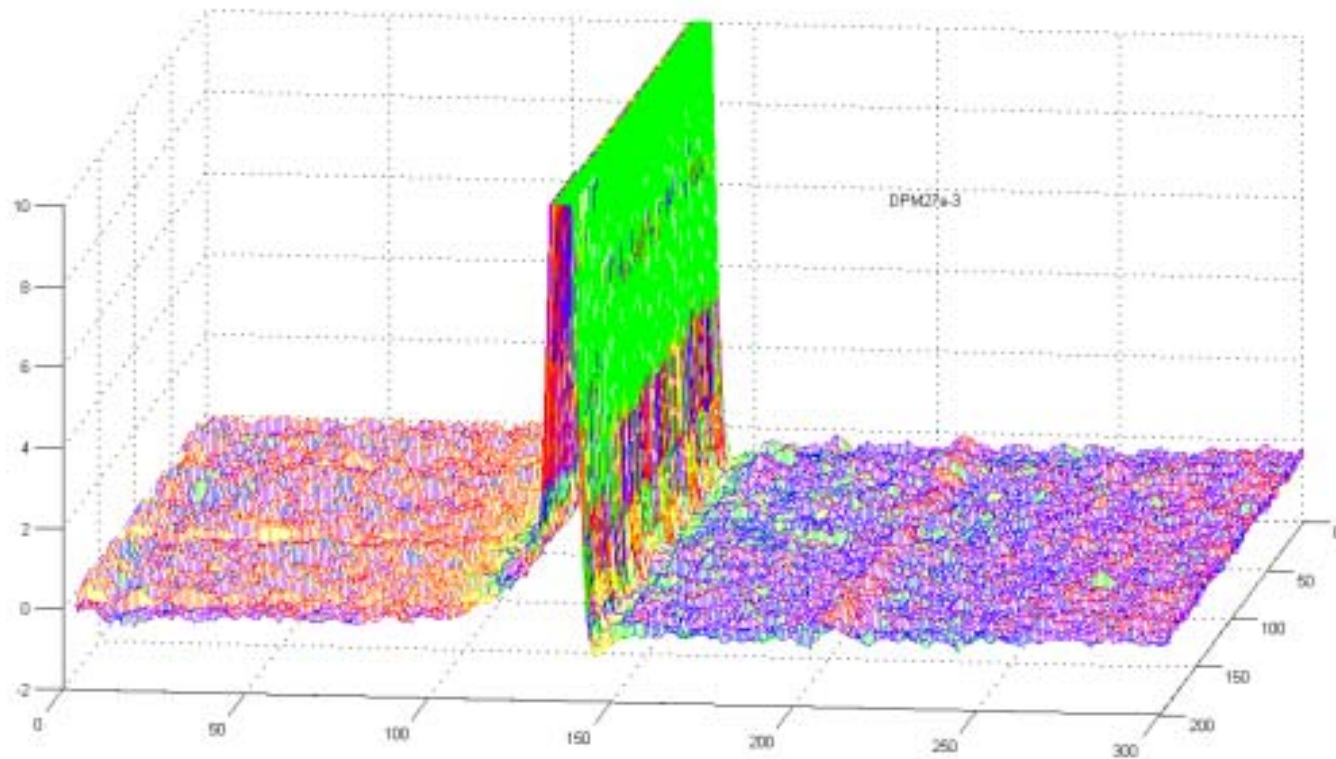


Typical IMS Signature: Positive Cell



DPM from Confidence Tube

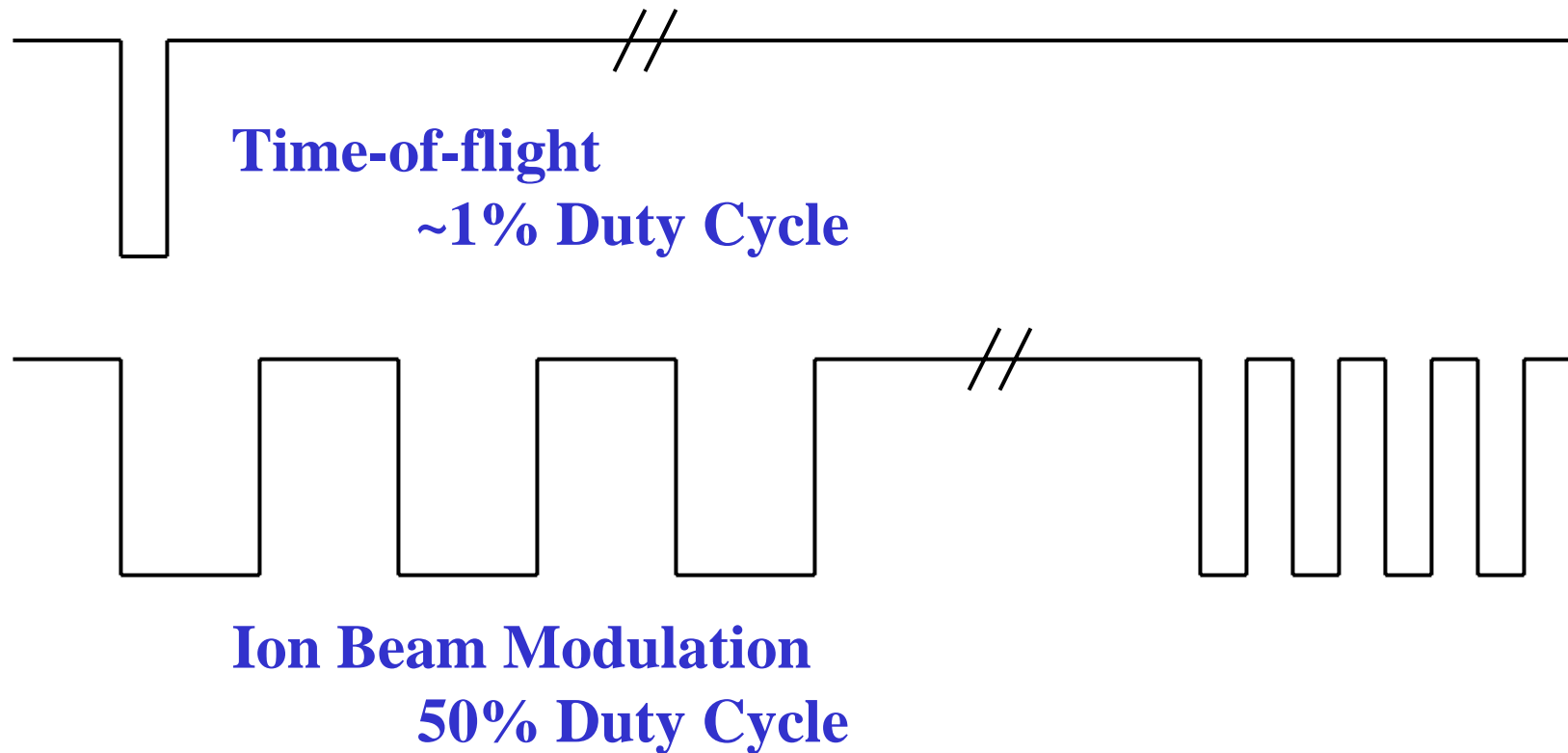
IMS Response at Low Concentration



0.027 mg/m³

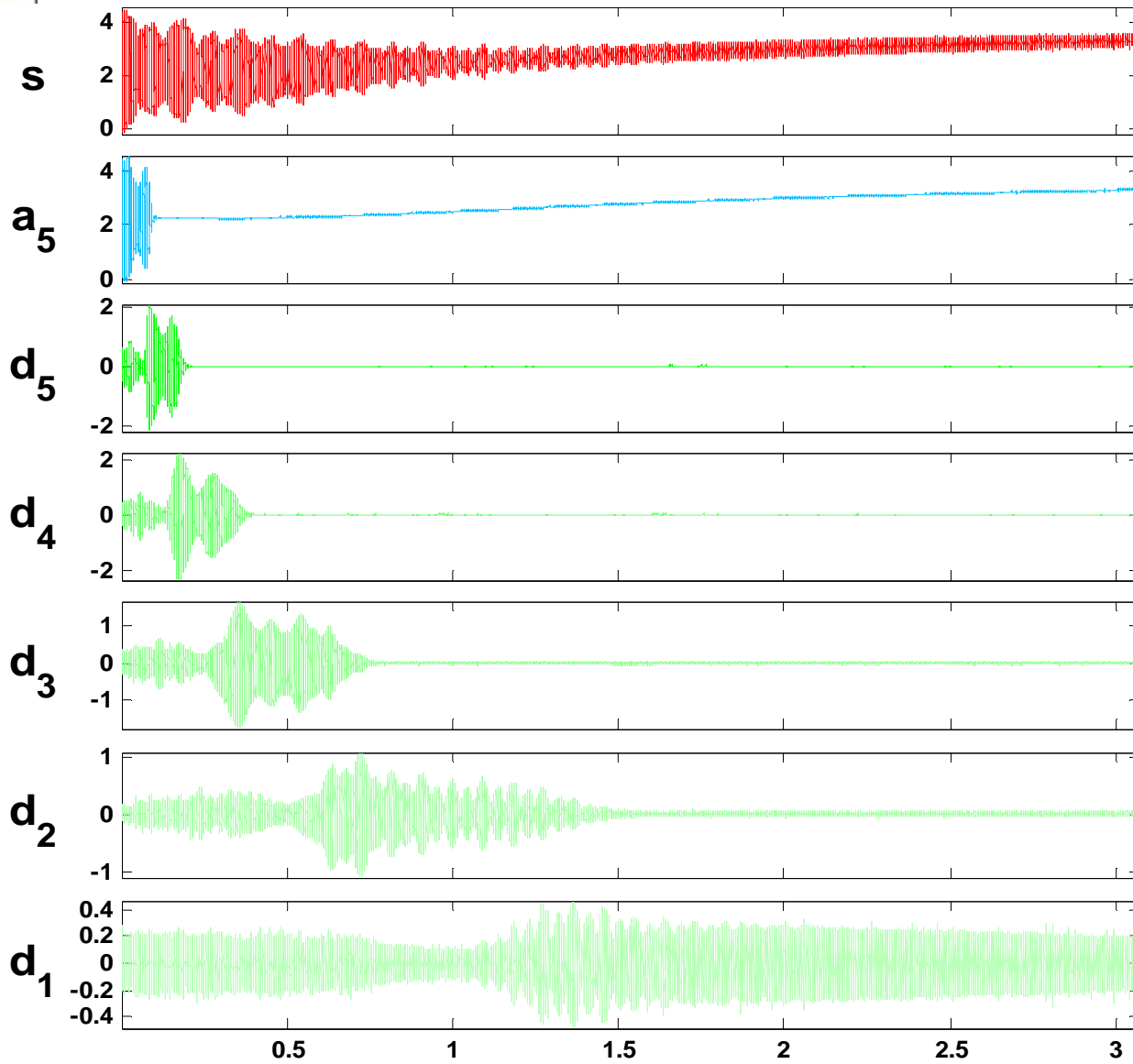


BNG Driver Timing



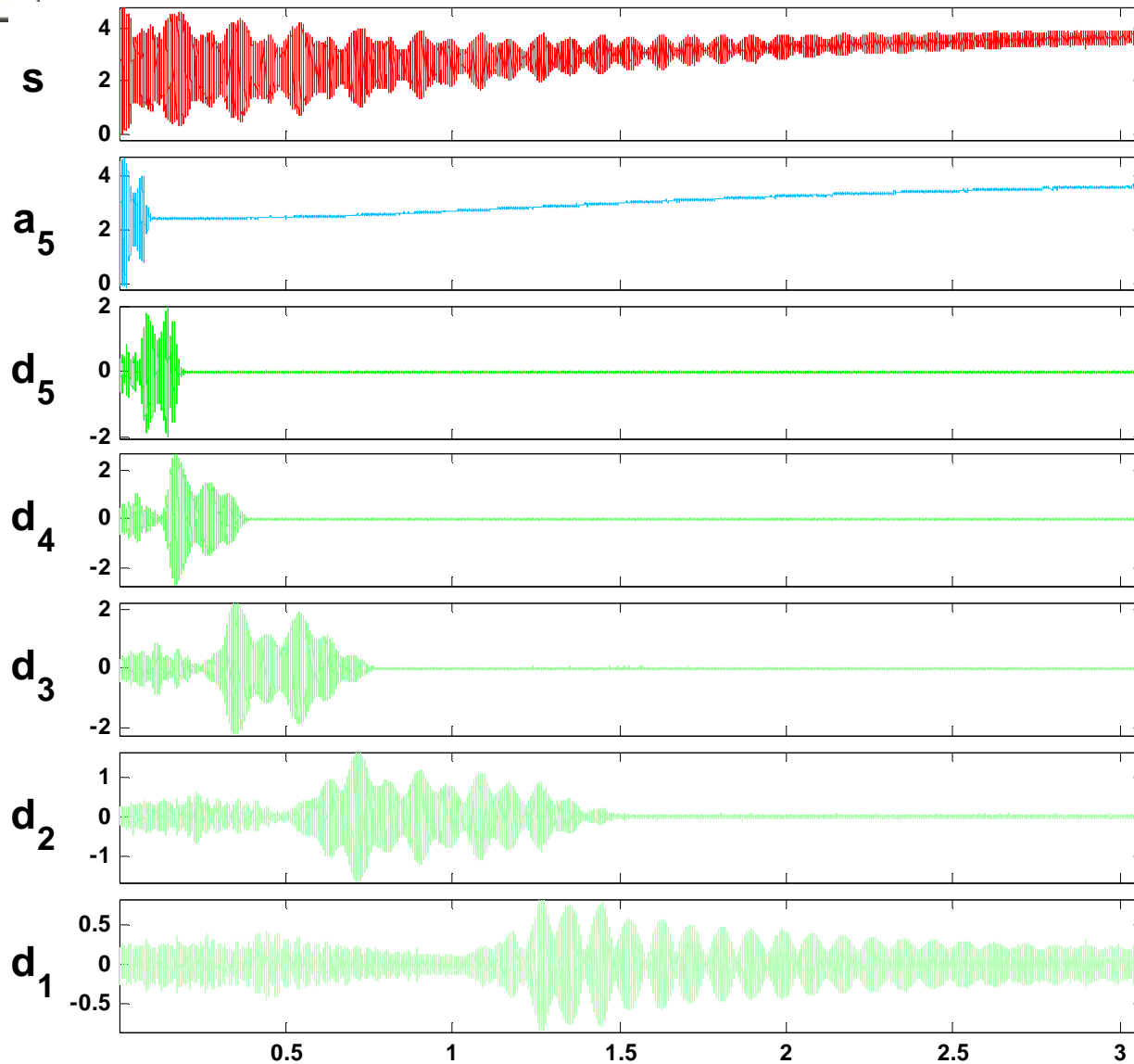
Wavelet Decomposition

Background

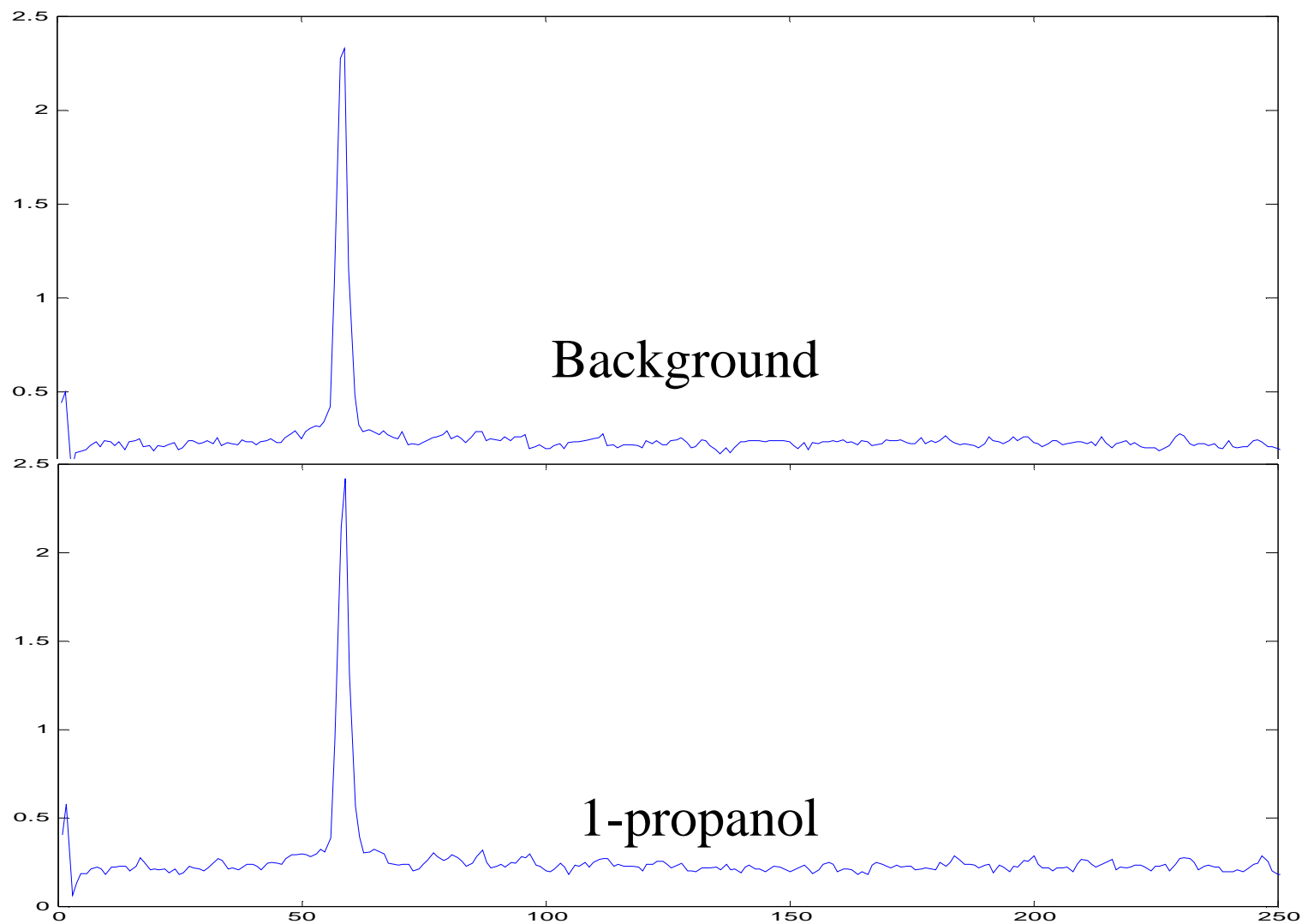


Wavelet Decomposition

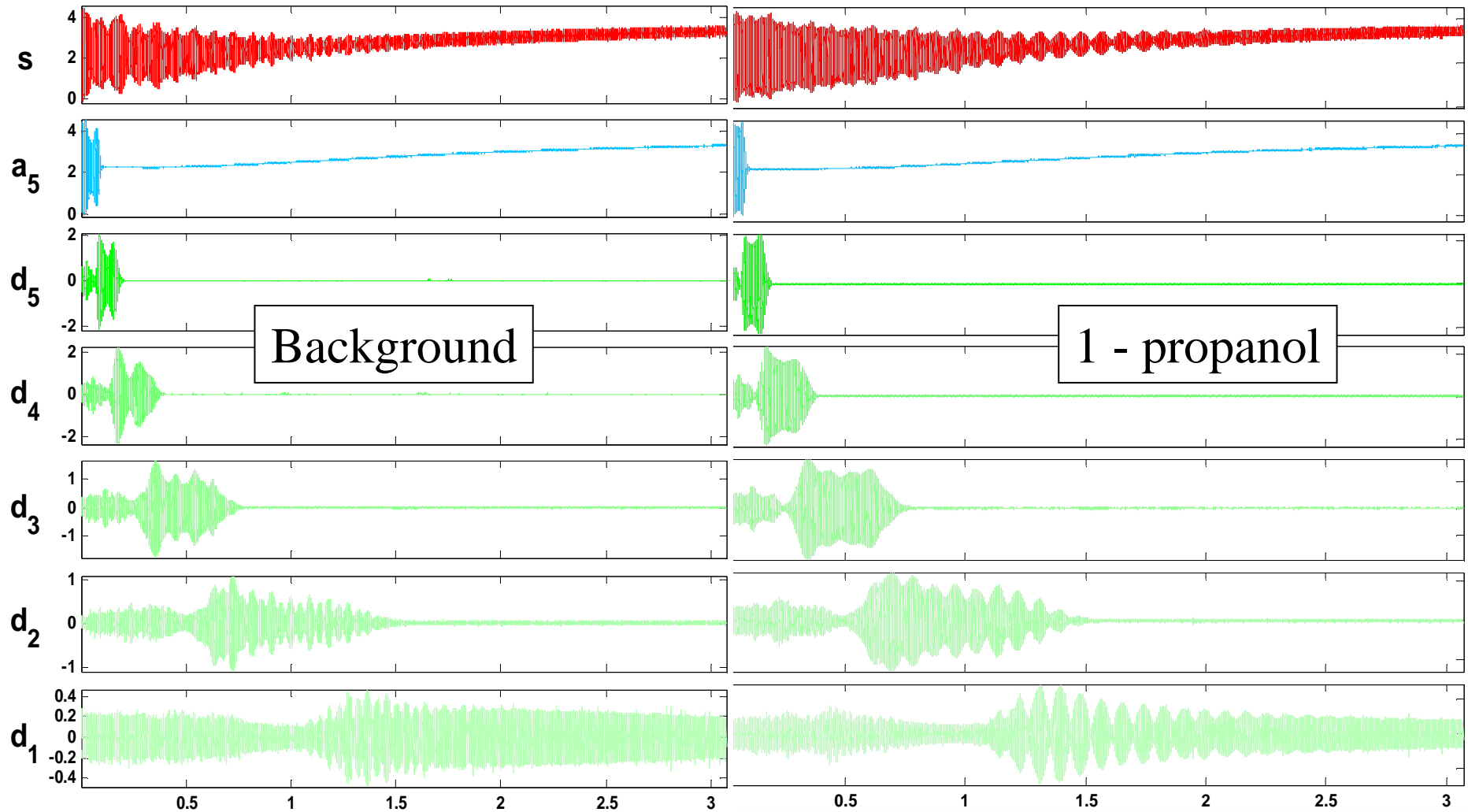
DPM



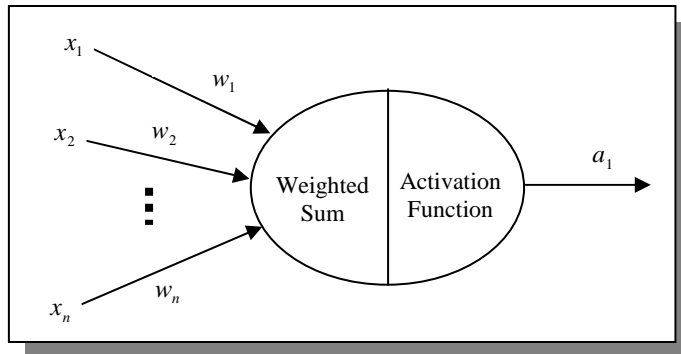
Time-of-flight Measurement



Wavelet Decomposition

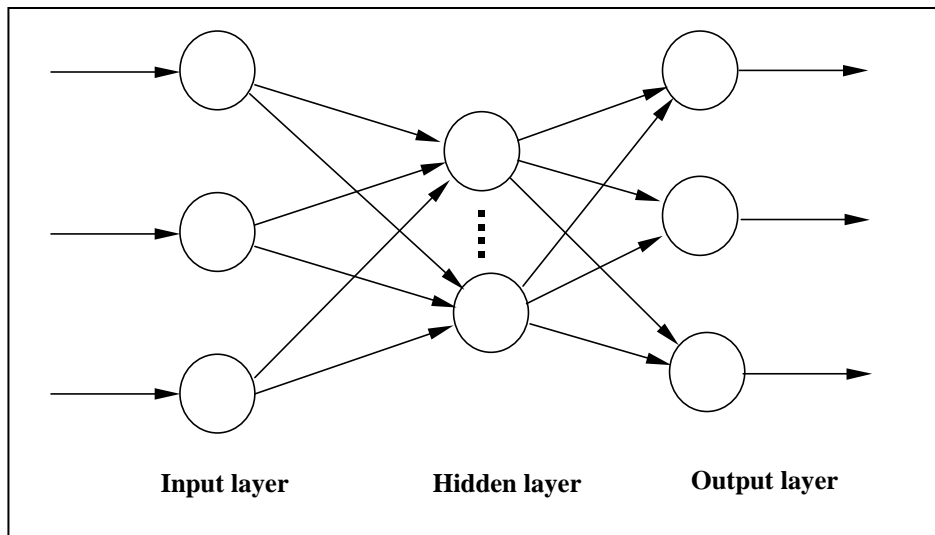


Neural Networks



Adaptive Learning Rule:

$$W^{new} = W^{old} + (t - a) \bullet X^T$$



- Benefit of Multi-layered NN: They can approximate any function
- Difficulty: Updating weights in the hidden layers
- Solution: **Back-propagation of error**

– Gradient Descent:

$$\Delta W = -\eta \frac{\partial E}{\partial W}$$

$$E = \frac{1}{2} \sum_i (t_i - a_i)^2$$

$$a_1 = f(x_1 w_1 + x_2 w_2 + \Lambda + x_n w_n) = f\left(\sum_{i=1}^n x_i w_i\right) = f(W^t T)$$





Results

- Collected data sets using ion beam modulation
 - Background
 - DPM
 - 1-propanol
- Performed Wavelet Decomposition
- Used 5 new statistical evaluators
- Trained 5-node Neural Network (Feed forward)

Analyte	Results	% Correct
Background	3/3	100%
DPM	5/5	100%
Propanol	3/3	100%



Conclusions and Future Work

- Wavelets can help improve S/N
 - Wavelets can be used to decompose signal for further analysis
 - Ion beam modulation improves selectivity and sensitivity
 - Neural networks can be used to detect modulated ion beam data
-
- Investigate modulation schemes
 - Determine algorithm robustness
 - Decrease IBM scan time
 - Decrease IBM data acquisition rate
 - Expand training sets
 - Look at other metrics (cell temperature, humidity)





Acknowledgements

Funding:

Integrated Detection of Hazardous Materials (IDHM) Program, a Department of Defense project managed jointly by Center for Sensing Science and Technology, Purdue University, and Naval Surface Warfare Center, Crane, Indiana.

Collaborators:

Rong Gao*, Lefteri H. Tsoukalas
Applied Intelligent Sensing Lab (AISL)
School of Nuclear Engineering, Purdue University
West Lafayette, IN 47907

